Poster III-66

Computational Biology and Medicine at CFD Research Corporation

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Advances in theoretical biology have made possible the formulation of detailed mathematical models of many basic mechanisms associated with coupled biological interactions. We are currently developing and implementing a range of such models into our coupled multidisciplinary simulation software CFD-ACE+. The resultant simulation tools have allowed us to perform *in-silico* studies ranging from investigations of basic bio-dynamics to treatment planning. This presentation illustrates some varied aspects of the simulation-based biological research performed at CFD Research Corp.

a) Tumor-Induced Angiogenesis Modeling: We are developing computational software for modeling of angiogenic processes induced by solid tumors. Direct applications include the analysis of drug delivery to the tumor, treatment prototyping, and theoretical investigations of angiogenesis and tumor dynamics. We have conducted simulations on quasi 3D and fully 3D domains to study vasculature formation, as well as effects of anti-angiogenic factors on vasculature development, drug delivery and solid tumor response. This research was sponsored by NIH SBIR Phase I Grant # R43 CA 97827-01.

b) Coupled Simulations of Cellular Biophysics: Our current work in this area includes first-principles modeling of dynamics of immune synapses, bacillus subtillis cell division, and dynamics of E-coli bacterial chemotaxis. We are also developing and implementing detailed models of metabolic and signaling pathways. This work includes yeast cell-cycle dynamics, chemosensing and chemotaxis pathways, and macroscopic bacterial behavior during infection. This research is being sponsored by DARPA SBIR SimBiosys Phase II Contract #MDA-972-02-C-0017 and DARPA BioSpice Project under Subcontract #6513845 to UC Berkeley.

c) Image/Model Based Treatment Planning: We are simulating the effect of etidiazole diffusion from a wafer in realistic 3D tumor geometry as a part of drug delivery study. The geometry was obtained from raw dicom data transferred into grid generation formats. In related work focusing on the effective heat impact due to RF magnetics in cancer therapy, we are simulating the temperature field evolution and corresponding voltage requirements for an RF catheter used in localized tumor ablation therapy.

d) Simulation of Vascular Devices: We have developed models coupling chemistry, structural mechanics, and hemodynamic factors as part of our research in the area of implantable vascular treatment. Our current work includes detailed coupled structural and fluid simulations of the elution of drugs from coated stents.

e) Hydrodynamic Protein Models: We have developed reduced protein bead models for evaluating the hydrodynamic properties of protein molecules by fitting the SAXS profile. Protein PDB data is used. The results show that such reduced models can greatly accelerate the simulations without degradation in accuracy.